

MARS SURFACE GAS DIFFUSION STUDY

Final Progress Report

27 May 1968

09514-6008-R000

Prepared for:

California Institute of Technology

Jet Propulsion Laboratory

Pasadena, California

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ABSTRACT

The soft landing of a spacecraft on the surface of Mars will result in a flow of heat and exhaust gases into the soil. The results of an analytical study on these transport phenomena are presented in this final report.

General governing equations for heat and mass transport in a porous medium are established. The equations are then reduced to forms which best describe the flow of heat and exhaust gases into the Mars soil and for which closed form solutions can be obtained. Approximate boundary conditions selected with regards to the rate of descent and engine cut-off height of the spacecraft are utilized to obtain specific solutions. A value of the thermal diffusivity is used which best accounts for the soil type, gas pressure and temperature expected on the Mars surface. Multipomponent diffusion theory can not be applied to the diffusion processes encountered here, and an effective binary diffusion coefficient is therefore used in the equations governing exhaust gas diffusion into and out of the soil. Adsorption and subsequent desorption of exhaust gases by the Mars soil may occur. However, the lack of data on adsorption and desorption rates precludes a concise analysis of these effects.

CONTENTS

	Page
1. INTRODUCTION	1
2. GENERAL THEORY AND BASIC EQUATIONS	3
2.1 Energy Transfer - Mass Coupling	3
2.2 The Governing Equations	4
2.3 The Equations Governing Heat and Mass Flow into the Mars Soil	6
3. TEMPERATURE PROFILES AND EXHAUST GAS CONCENTRATION WITHIN THE MARS SOIL	12
3.1 Designation of the Near Field and Far Field Regions on the Mars Surface	12
3.2 Near Field Analysis	14
3.3 Far Field Analysis	15
3.3.1 Boundary and Initial Conditions for Gas Flow	15
3.3.2 Boundary and Initial Conditions for Heat Flow	19
3.3.3 Values of the Transport Parameters	19
3.3.4 Specific Solutions to the Heat Transfer and Diffusion Equations	25
3.3.5 Simultaneous Diffusion and Adsorption	32
4. SUMMARY AND RECOMMENDATIONS	36
5. REFERENCES	39

1. INTRODUCTION

Plans are presently being formulated for soft landings on the surface of Mars by unmanned spacecraft carrying scientific instruments. Such a spacecraft will be able to collect and transmit to Earth considerable data that will help to answer many questions concerning the conditions on the surface of Mars. Even though astronomers have been obtaining data on Mars for many decades, considerable uncertainty yet remains concerning such factors as the chemical composition and pressure of the atmosphere, soil composition, surface temperature, and the possibility of simple forms of life on Mars. Astronomy is simply not capable of answering all the questions relating to Mars which scientists are raising - hence the need for a soft landing spacecraft on the surface of Mars to collect data.

Precautions, however, must be taken to assure that the information obtained by the spacecraft instruments truly represents the conditions on the surface of Mars. Thus, one must bear in mind that the spacecraft itself may perturb the local surface conditions and affect the data collection. The study reported herein is concerned with several aspects of local surface "contamination" by the spacecraft. In particular, the study is directed toward predicting, analytically, the degree of soil heating by the exhaust gases and the quantity of mass flow of exhaust gases into the soil with any possible simultaneous chemical reactions. With time history predictions available for the temperature distribution and the exhaust gas distribution within the soil, those responsible for designing the spacecraft soil experiments will be able to consider the possible effects of the exhaust gases upon the soil. Also, after the experiments have been conducted and the data transmitted to Earth, the data interpretation can be performed in the light of the predicted effects of the exhaust gases.

Consider the nature of the exhaust gas - soil interaction phenomena. The Mars surface will be exposed for a short period of time to hot, high velocity exhaust gases from the retro-rockets of the descending spacecraft. The exhaust gases will tend to heat the soil surface (heat also may be transferred to the soil by radiation directly from the hot rocket engine) thereby causing a heat flux into the soil. Also, as the gases flow over the soil surface, a fraction of the gases will flow into the soil pores and displace the atmospheric gases initially there. After the rocket engine cuts off, the soil will begin to cool, and the exhaust gases will gradually be redisplaced in the soil pores by the

atmospheric gases. These transient exhaust gas-soil interaction processes may be analyzed by the theory of heat and mass transfer in porous media. That is, simultaneous equations can be written which govern the transport of heat and gases in soils. However, as will be seen in the following chapters, the exact equations prove far too complex for solutions to be obtained. Reasonable simplifications, based on the physics of this particular heat and mass transfer problem, can be made in the theory, and the governing equations made amenable to solution.

Contamination studies have been previously performed for spacecraft landings on the lunar surface. Aronowitz, et al, (1) conducted an extensive study on the effects of a LEM descent engine on the surface of the Moon. Soil erosion, atmospheric contamination, soil contamination, and chemical reactions that may result in a moon landing were investigated. Flow of exhaust gases into the soil was, however, not studied. Hutton (2) considered the surface erosion (cratering) that will result upon a soft landing on Mars. No work, however, has been performed prior to the study reported herein which is directed at obtaining a prediction of the heat transfer and exhaust gas flow into the Mars soil.

2. GENERAL THEORY AND BASIC EQUATION

2.1 Energy Transfer - Mass Transfer Coupling

The exhaust gas-soil interaction problem, as briefly discussed above, is basically a simultaneous energy and mass transfer phenomena. Mass transfer refers to the flow of exhaust gases and atmospheric gases into and out of the Martian soil. Energy transfer refers to the heat transfer to the soil and to the thermal energy liberated (or adsorbed) by chemical reactions between the exhaust gases which flow into the soil and the soil constituents. The two processes - energy transfer and mass transfer - do not proceed independently of one another.

Consider the physics of the energy transfer process. Thermal energy, heat, is conducted into the soil because the soil surface is heated by radiation from the hot rocket engine and by the hot exhaust gases sweeping over the surface. Also, heat is convected into the soil by those exhaust gases which flow into the soil. Then, heat can be liberated within the soil by chemical reactions which occur between exhaust gases and the soil constituents. Therefore, a portion of the energy transfer into the soil, the convected heat and the heat from chemical reactions, is dependent upon the extent of the exhaust gas flow (the mass transfer process) into the soil.

Mass transfer into and out of the soil occurs due to changes in total gas pressure and/or component concentrations at the surface. However, it is also known that temperature differences (temperature gradients, strictly speaking) may cause mass diffusion. That is, even in the absence of total or partial pressure gradients, mass diffusion may occur if temperature gradients are present. Mass transfer due to total and partial pressure differences (such as arise when the exhaust gases sweep across the surface), is also dependent on the soil temperature distribution because the parameters which govern the pressure induced flow, such as the gas viscosity and the diffusion coefficients, are slightly temperature dependent. To summarize, the point to be made is that the energy and mass transfer processes that occur during the landing of a retro-rocket powered spacecraft on Mars are coupled to some degree. The two processes must be mathematically analyzed as coupled processes in order to obtain exact solutions for the temperature distribution and the exhaust gas distribution within the Mars soil.

The exact solutions referred to above are, in most energy and mass transfer problems, nearly impossible to obtain. General differential equations may be established, but solutions seldom are obtained due to the nonlinearities and complexities of the equations. Unfortunately, this is the case in the present study of the exhaust gas-Mars soil interaction. Although an exact solution reflecting the mass transport-energy transport coupling can not be obtained, adequate engineering solutions can be obtained by utilizing simplified governing equations. It is the purpose of this chapter to discuss the general governing equations and to indicate the simplifications necessary for a solution.

2.2 The Governing Equations

General equations governing mass and energy transport in multicomponent systems are obtained by combining mass and energy conservation equations with equations expressing the mass and energy fluxes in terms of transport properties and gradients of temperature and specie concentrations. Bird, Stewart and Lightfoot (3) point out that the governing equations may be written in many forms depending on whether D/Dt or $\partial/\partial t$ is used, which reference frame is selected for the fluxes, whether mass or molar units are used, and how the various forms of energy are broken up. No useful purpose will be served by a detailed discussion of these many various forms, but a presentation of selected equations will aid in explaining the final approach used in this study.

A mass conservation equation of the form, for example,

$$\frac{\partial}{\partial t} \rho_i = - \nabla \cdot \bar{J}_i + r_i, \quad i = 1, 2, \dots, n \quad (1)$$

is needed for each of the n components of the multicomponent mixture, where ρ_i is the density of the i^{th} component, \bar{J}_i is the mass flux vector of the i^{th} component with units of mass per unit time, and r_i is the chemical reaction source term (3).

The conservation of energy expression may be written as

$$\frac{\partial}{\partial t} \rho \left(U + \frac{1}{2} v^2 \right) = - (\nabla \cdot \bar{e}) + \sum_{i=1}^n (\bar{J}_i \cdot \bar{g}_i) \quad (2)$$

where U is the specific potential energy, $(1/2)v^2$ is the specific kinetic energy, \bar{e} is the energy flux vector, and \bar{g}_i is the external body force on the i^{th} component. Note that the mass flux vector \bar{J}_i occurs in both conservation equations.

In order to obtain differential equations that can be solved for the temperature and specie concentration distributions, the fluxes \bar{j}_i and \bar{e} in equations 1 and 2 must be replaced by expressions that contain the transport properties and the gradients of the concentration and temperature. The expression for the fluxes can not be written in the concise, exact manner of equations 1 and 2. That is, empirical flux relations are often necessary. The flux expressions are best obtained through the theory of nonequilibrium thermodynamics (4) which relates the fluxes to gradients of the intensive parameters (such as the gradients of the temperature and component concentrations) through proportionality constants (such as the thermal conductivity). Consider the expression for the flux of the i^{th} ideal gas in a mixture of n ideal gases at a uniform temperature and total pressure and in the absence of external mechanical driving forces. For these conditions the diffusion flux of the i^{th} gas is given as

$$\bar{j}_i = -\rho \sum_{j=1}^n D_{ij} \nabla c_j \quad (i = 1, 2, \dots, n) \quad (3)$$

where ρ is the total density, D_{ij} are multicomponent diffusion coefficients*, and c_j are mass fractions of the n gases. When temperature and pressure gradients exist in the system, additional terms must be added to the right hand side of equation 3. For example, a temperature gradient results in a mass flux given as (4)

$$\bar{j}_i = -\rho c_i D_i^t \nabla T \quad (4)$$

where D_i^t is the thermal diffusion coefficient. Note, therefore that the mass flux vector of each constituent depends on the gradients of all constituents and on temperature and pressure gradients as well.

*Nonequilibrium thermodynamic theory establishes the conditions for which $D_{ij} = D_{ji}$. If the driving force is properly chosen, then $D_{ij} = D_{ji}$. In equation 3, ∇c_j is the driving force for mass flow, but it does not satisfy the requirements of nonequilibrium thermodynamics in order that $D_{ij} = D_{ji}$. Therefore, for each diffusing constituent of the mixture, n diffusion coefficients must be known to exactly specify the mass flux when the driving forces are the specie concentration gradients, ∇c_j .

The expression for the general flux vector \bar{e} of equation 2 also has several terms. Perhaps the most simple form of the energy flux vector is $\bar{e} = \bar{q} = -k\nabla T$, which is Fourier's law of heat conduction and is valid only for zero mass flow. When mass flow also occurs, an additional term must be added to the energy flux vector to account for the energy transported by the convected mass.

Substituting the mass and energy flux expressions into the conservation equations 1 and 2, one obtains, in general, a set of nonlinear differential equations. These equations, along with the proper boundary and initial conditions, must be solved for exact solutions to the temperature distribution and specie concentration distributions problem. However, exact solutions to such a set of differential equations are usually difficult to obtain, and simplifications and approximations to the equations can often be made which allow for a much less difficult solution and affect the accuracy of the solution to only a small degree. The next section considers the reduction of the general differential equations to a set of equations which accurately, but not exactly, describe the exhaust gas-soil interaction phenomena yet for which solutions can be obtained.

2.3 The Equations Governing Heat and Mass Flow into the Mars Soil

In this section the equations governing the flow of heat and mass into the Mars soil will be obtained from within the framework of the general theory presented in the previous section. Solutions of these equations for specific values of the various pertinent parameters and boundary conditions will be presented in the following chapter.

Consider first the heating of the Mars soil. Sources of thermal energy at a point below the soil surface are: (1) heat conducted through the soil from the surface, (2) heat convected by the gases flowing into the soil, and (3) heat generated (or absorbed) by chemical reaction. The energy conservation equation may be written as

$$\rho c_p \frac{\partial T}{\partial t} = -\nabla \cdot \bar{q} + G \quad (5)$$

where ρ is the soil density, c_p is the soil specific heat, \bar{q} is the heat flux vector and G is the heat generation term. The heat flux vector may be expressed as

$$\bar{q} = -k \nabla T + h \bar{j} \quad (6)$$

where k is the thermal conductivity of the soil, \bar{j} is the mass flux of gas into the soil, and h is the specific enthalpy of the gas*. If the convected heat term $h \bar{j}$ can be shown to be small compared to $-k \nabla T$ and if the heat generation term G is negligible, substitution of $q = -k \nabla T$ into equation 5 results in the well known equation

$$\rho c_p \frac{\partial T}{\partial t} = k \nabla^2 T \quad (7)$$

where k is assumed constant. Exact solutions to equation 7 are readily obtained for many boundary and initial conditions. Thus, by neglecting the contribution of the mass flux to the heat transfer process, one "decouples" the heat transfer equation from the mass flow equations. If the mass flux heat transfer term $h \bar{j}$ can not be dropped from equation 6, then upon substitution of \bar{q} into equation 5 one obtains an expression which still contains a mass flux term \bar{j} . One must then resort to using an expression such as equation 3 in order to relate \bar{j} to the independent variables of the problem. The end result is an equation for which a closed form solution probably can not be obtained.

For the case of low density gas diffusing into the Mars soil, it is reasonable to assume that the heat convected by this gas is small compared to the heat conducted by the soil. Calculations presented in a following section verify that a small total mass of gas diffuses into the soil. Also, since no chemical reactions between the exhaust gases and the soil components appear likely**, the heat generation term may be assumed to be zero. Therefore, equation 7 accounts for the primary source of energy transfer within the Mars soil, and solutions of this equation will yield accurate predictions of the temperature distributions within the soil. Proper values of ρ , c_p , and k of the soil as well as the necessary boundary and initial conditions are discussed in Chapter 3 prior to presenting the solutions of the equation.

*The specific enthalpy of an ideal gas is $c_p T_g$ where c_p is the gas specific heat and T_g is the local gas temperature. For gas flow into the soil, the gas temperature at a point does not necessarily equal the local soil temperature at the same point.

**Additional discussion to follow.

Now consider the problem of describing the exhaust gas flow into the porous Mars soil by equations for which solutions can be reasonably obtained. The exact, rigorous approach was previously presented. The conservation equation, equation 1, is written for each component of the multicomponent exhaust gas mixture. Then, expressions relating the chemical reaction term r and the mass flux term $\nabla \cdot \mathbf{j}_i$ to the independent variables of the problem (the concentrations, temperature, etc.) must be substituted into the conservation equation in order to obtain the differential equations which can, theoretically, be solved for the concentration distributions within the Mars soil. For practical engineering solutions, however, simplifications must be made.

First, since chemical reactions between the rocket exhaust gases and the Mars soil do not appear probable, the chemical reaction term r of equation 1 may be assumed zero*. It is fortunate that no large scale chemical reactions are likely since the term r is generally greatly dependent upon temperature, concentration, and pressure for any chemical reaction. Inclusion of such a term in equation 1 would make for a difficult solution.

Secondly, the expression for the mass flux $\bar{\mathbf{j}}_i$ can be simplified considerably for the case of exhaust gas flow in the Mars soil. As previously indicated $\bar{\mathbf{j}}_i$, the mass flux of the i^{th} component of a multicomponent gas mixture, depends on the concentration gradients of all the mixture constituents as well as the pressure and temperature gradients. Equation 4 expresses the contribution to $\bar{\mathbf{j}}_i$ resulting from the temperature gradient, but as pointed out this term is normally small and will be neglected. Assuming negligible thermal diffusion, the gas flow in the porous Mars soil will be due solely to concentration gradients and/or to the total pressure gradient.

It will be shown in the next chapter (when boundary conditions for the governing equations are formulated from the expected actual surface conditions) that the Mars surface area subjected to the exhaust gases can be divided into two regions based on the flow regimes within the soil. Gas flow in the soil of the two regions will be governed by different equations. In the region directly beneath the engine exhaust nozzle, the total pressure at the soil surface will be great enough to establish a total pressure gradient within the soil thereby causing a bulk gas flow. The velocity of fluid flowing in a porous medium subjected to a total pressure** gradient is given by Darcy's law (3),

*A particular case for r independent of temperature but not zero will be discussed in a following section.

**The total pressure repeatedly referred to is the sum of the partial pressures of the gases in the multicomponent mixture.

$$v_o = - \frac{k}{\mu} \nabla p \quad (8)$$

where v_o is the superficial velocity (volume rate of flow through a unit cross-sectional area of the solid plus fluid) averaged over a small region of space - small with respect to microscopic dimensions in the flow system but large with respect to the pore size, k is the permeability of the porous medium, and μ is the fluid viscosity. The mass flux may be written as

$$j = \rho v_o = - \frac{\rho k}{\mu} \nabla p \quad (9)$$

where ρ is the fluid density.

Equation 9 is substituted into a modified mass conservation equation

$$\epsilon \frac{\partial \rho}{\partial t} = - \nabla \cdot j$$

where ϵ is the porosity of the porous medium (ϵ is defined as the ratio of pore volume to total volume) in order to obtain the equation

$$\frac{\epsilon \mu}{k} \frac{\partial \rho}{\partial t} = \nabla \cdot \rho \nabla p \quad (10)$$

Equation 10 and the equation of state of the fluid describe the motion of a fluid in a porous medium. For example, if one assumes an incompressible liquid, $\rho = \text{constant}$, equation 10 reduces to Laplace's equation $\nabla^2 p = 0$. However, for gases the expansion process influences the form of the resulting equation. For example if an isothermal gas flow process occurs, the equation of state $p = \rho RT$ and equation 10 yield

$$\frac{2\epsilon\mu\rho_o}{k} \frac{\partial \rho}{\partial t} = \nabla^2 \rho^2 \quad (11)$$

where ρ_o is the gas density at unit pressure.

Equation 11, therefore, governs the transient gas flow in the Mars soil in any region where a significant total pressure gradient exists in the soil and when the flow is assumed isothermal. As indicated, it will be shown that this equation may be used to describe the flow for the soil region near the surface stagnation point of the exhaust gas flow field.

An equation will now be obtained for the flow of gases in the region of the Mars soil where total pressure gradients are small but where significant concentration gradients of the individual gases exists. The surface region thus affected will be the region swept over by exhaust gases that have a pressure at the surface equal to the ambient Mars atmospheric pressure. Since no total pressure gradient exists, no bulk flow (Darcy's law flow) will occur. However, the exhaust gas multicomponent mixture at the soil surface differs from the mixture of gases initially within the soil (i.e., the gases comprising the Mars atmosphere). Therefore, concentration, or partial pressure, gradients exists for each gas present, and interdiffusion of the gases will proceed governed by equation 3, $\bar{J}_i = -\rho \sum_{j=1}^n D_{ij} \nabla c_j$ applied to each of the n gases*. Since five gases comprise the exhaust mixture (CO , CO_2 , H_2 , H_2O , N_2), and under the assumption that the Mars atmosphere is primarily nitrogen, one obtains six equations of the form of equation 3. Each equation contains six terms each with a different diffusion coefficient. For $n > 2$, the quantities D_{ij} and D_{ji} are not in general equal (3), therefore 36 different diffusion coefficients will appear in the six equations. Diffusion coefficients have reportedly been calculated for simple steady state diffusion problems involving a three component mixture, but for the case of six gases interdiffusing in the Mars soil no practical way exists to calculate all of the required diffusion coefficients.

An alternative mathematical description is available which considerably simplifies the multicomponent diffusion process. It is convenient to define an effective binary diffusivity D_{im} for the diffusion of the i^{th} gas in a mixture. The multicomponent diffusion problem is thereby reduced to a binary diffusion problem which assumes that any one gas component diffuses into the remaining gas mixture as if the mixture were a single component. Bird, Stewart, and Lightfoot (3) point out that for some special kinds of diffusing systems the expression for D_{im} becomes particularly simple, namely:

Case a - For trace components 2,3,...n in nearly pure species 1, $D_{im} = D_{i1}$

Case b - For systems in which all the D_{ij} are the same, $D_{im} = D_{ij}$

*It is assumed here that any temperature gradient which exists is small since equation 3 is strictly valid only for a zero temperature gradient.

It will be shown in the next chapter, when specific values of diffusion coefficients are considered, that all the D_{ij} should be approximately the same for gas diffusion in the Mars soil. Therefore, according to case b it will be valid for this study to let D_{im} equal D_{ij} . It is also pointed out (1) that this approach to solving multicomponent problems seems to give good results for calculating mass transfer rates but a less satisfactory quantitative description of concentration profiles. In the absence of any alternative procedure, the D_{im} approximation has been used in this study to predict the concentration profiles of the exhaust gases in the Mars soil.

Combining the conservation equation, equation 1 and equation 3 written for the i^{th} gas in a mixture m one obtains

$$\frac{\partial c_i}{\partial t} = D_{im} \nabla^2 c_i \quad (12)$$

where c_i is the mass fraction ρ_i/ρ .

Solutions to equation 12 represent the desired concentration profiles in the Mars soil. These solutions, utilizing proper values of D_{im} in conjunction with initial conditions and boundary conditions for the mass fractions c_i , are presented in Section 3.2.3.

Equation 12 may be modified to account for adsorption and desorption of the i^{th} gas by the soil. An approximate solution is presented in Section 3.2.4 for the equations

$$\frac{\partial c_i}{\partial t} = D_{im} \frac{\partial^2 c_i}{\partial x^2} + \lambda_d c_{di} - \lambda_c c_i \quad (13)$$

$$\frac{\partial c_{di}}{\partial t} = \lambda_c c_i - \lambda_d c_{di} \quad (14)$$

where c_{di} represents the quantity of i^{th} adsorbed constituent, $(\lambda_d c_{di})$ is the rate of desorption, $(\lambda_c c_i)$ is the rate of adsorption. Note that the combined term $(\lambda_d c_{di} - \lambda_c c_i)$ is actually a chemical reaction term r such as in equation 1. In this present section on the development of equations governing gas flow into the Mars soil, r has been assumed zero because chemical reactions generally do not appear probable.

3. TEMPERATURE PROFILES AND EXHAUST GAS CONCENTRATIONS WITHIN THE MARS SOIL

3.1 Designation of the Near Field and Far Field Regions on the Mars Surface

Differential equations have been established which govern the heat flow and exhaust gas flow into the Mars soil. These equations, however, do not describe the gas flow field above the soil surface. The problem of exhaust gases issuing from a rocket engine, spreading over the Mars surface and interacting with the low pressure atmosphere is a complex compressible flow gas dynamics phenomenon. A study of the above surface flow field is not included in this report. Experimental and analytical efforts in this area are presently being supported by Jet Propulsion Laboratory, but final results are not yet completely available. The general nature of the exhaust flow field interaction with the soil surface is known, however. Since this above surface flow field is extremely important from the standpoint of determining proper initial conditions and boundary conditions necessary for the solution of the equations governing the heat and gas flow beneath the soil surface, some general aspects of this flow field will now be considered.

Figure 1 is a sketch of the expected flow field at some instant of time for a vertically descending rocket engine. The designation of "near field" and "far field" regions is of particular significance. The near field is that region where the surface pressure, static pressure plus the dynamic pressure component normal to the plane of the surface, is significantly above the ambient atmospheric pressure. Hutton's work (2) indicates that the near field extends from the surface stagnation point (denoted as S.P. in Figure 1) out to a maximum radius of approximately ten times the nozzle exit radius r_e^* . Beyond a radius of $10 r_e$, the surface is exposed to a radial flow of exhaust gases which have expanded to approximately the ambient atmosphere pressure. In the far field region the exhaust gases mix with the atmospheric gases until at some distance essentially no exhaust gases contact (and contaminate) the Mars soil surface. No analytical predictions have been made as to what this distance may be. However, Cox and Abbot (5) have experimented with a gas

*The extent of the near field depends on the height of the engine at the instant of time under consideration. The maximum radius of $10 r_e$ for the near field region occurs at the minimum engine cut-off height of 5 ft (2).

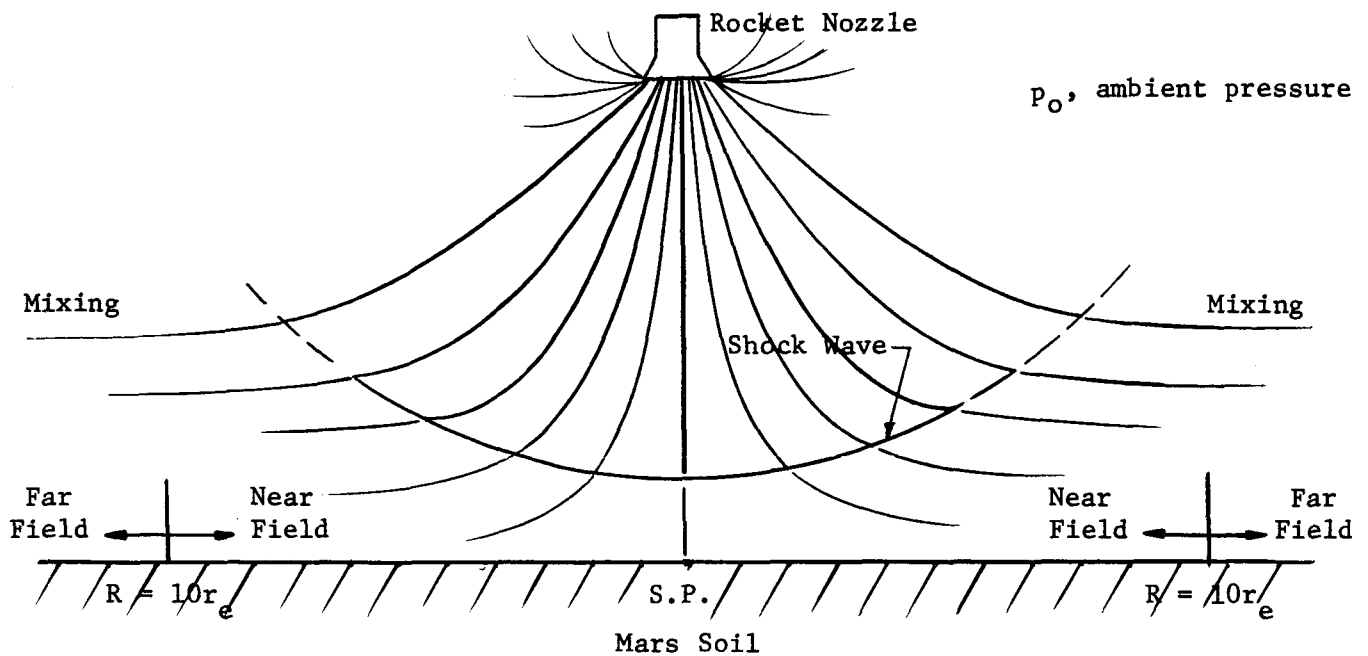


Figure 1 General features of the above-surface flow field

stream directed onto a horizontal surface and determined that eventually, as the radial flow slowed at large distances from the stagnation point, the buoyant forces caused the still warm flow stream to separate and rise from the surface. They obtained good agreement for the separation distance as the gas velocity, gas temperature, and nozzle height was varied. The data is plotted in nondimensional quantities. Their experimental variables, and the range, were: nozzle diameters - 1 and 2 inches; exit velocities - 50 to 1350 ft/sec; exit temperatures - ambient to 265°C ; ratios of nozzle diameter to the height above the surface - 1 to 36. The experiments were conducted in air at one atmosphere pressure. Therefore considering the range of variables, it is obviously questionable that an extrapolation of Cox and Abbot's curves will allow a reasonable prediction of the separation distance of the exhaust gases flowing across the Mars surface. However, the extrapolation required little effort, and using the spacecraft propulsion system parameters (temperature and velocity) from Hutton's report (2) along with a Mars atmospheric pressure of 10^{-2} Earth atmospheres and a value of gravity of 0.38 that on Earth, a separation distance of 450 ft minimum from the stagnation point was obtained. Due to the borderline nature of the extrapolation necessary to arrive at this distance, one should not be primarily concerned with the exact figure of 450 ft, but only with the order of magnitude. Thus, on this basis one may conclude that the far field area for this particular problem most likely extends beyond 10^2 ft from the stagnation point.

3.2 Near Field Analysis

The exhaust gas flow in the soil of the two regions (near field and far field) will be governed by different equations. The maximum surface pressure in the near field will be significantly above the atmospheric pressure* (the gases initially in the pores of the soil will, of course, be at the atmospheric pressure). With a total pressure gradient imposed upon the soil, a bulk flow of exhaust gases will occur first into the soil and then out of the soil after engine shut-down. Darcy's law must be utilized to describe such flow, and for isothermal permeation equation 11,

$$\frac{2\epsilon\mu\rho_0}{k} \frac{\partial\rho}{\partial t} = \nabla^2 \rho^2 \quad ,$$

describes the flow. Isothermal flow, except very near the soil surface, is a good assumption as will be seen after temperature profiles are considered. Equation 11 is a nonlinear differential equation for which no general solution exists. An unsuccessful attempt was made to solve the equation (with simplified initial and boundary conditions) by the method of similarity. This method employs transformations that reduce a partial differential equation to an ordinary differential equation for which a solution would have been very difficult to obtain. Even though a computer program to solve equation 11 is maintained by JPL, it was anticipated that excessive time would have been involved in obtaining and running the program for this problem. The near field surface is subjected to pressures which vary rapidly with time and radial distance from the stagnation point, and such boundary conditions often result in difficult computer solutions. Moreover, information concerning exhaust gas flow into the soil of the near field is not of major importance. That is, the spacecraft instruments will not likely be instructed to sample and analyze soil from the near field in order to determine the properties of virgin Mars soil. Therefore, in the light of the above facts, it was agreed to by JPL that this study need not include an analysis of the flow process in the near field.

*Hutton's results (2) show that at a nozzle height of 5 ft the surface pressure at the stagnation point is approximately four times the atmospheric pressure and at 5 r_e from the stagnation point the surface pressure is approximately twice the atmospheric pressure.

3.3 Far Field Analysis

3.3.1 Boundary and Initial Conditions for Gas Flow

The far field surface region is subjected to a negligible change (relative to atmospheric pressure) in total pressure by the radially flowing exhaust gases. However, exhaust gases tend to flow into the soil and displace the atmospheric gases initially present because concentration gradients are established and diffusion currents set up. As explained in Chapter 2, multi-component diffusion (the diffusion process in the far field) must be simplified to the binary diffusion case before the equations can be handled. Equation 12 utilizing the D_{im} simplification is therefore the best mathematical expression to use to describe the gas diffusion in the soil of the far field.

A degree of exhaust gas mixing with the atmospheric gases takes place, as previously discussed, as the exhaust flow proceeds radially outwards, and separation from the surface due to buoyant forces may occur at some radius. This mixing of the exhaust gases with the atmospheric gases should not cause the concentrations of the constituents of the exhaust gases to vary rapidly with radius from the stagnation point. This being the case, the term on the right hand side of equation 12 which accounts for a radial variation of c_i may be neglected (when expanded $\nabla^2 c_i$ includes the neglected term $\frac{1}{r} \frac{\partial}{\partial r} [r(\partial c_i / \partial r)]$ and the term $[1/r^2][\partial^2 c_i / \partial \theta^2]$ which is zero due to the axisymmetric nature of the flow). Equation 12 therefore reduces to the one-dimensional form,

$$\frac{\partial c_i}{\partial t} = D_{im} \frac{\partial^2 c_i}{\partial x^2} \quad ((15))$$

where x is the distance from the plane of the surface into the soil.

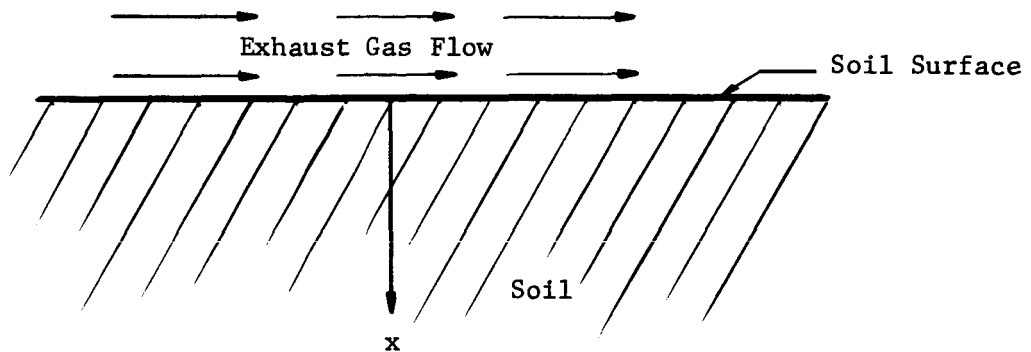


Figure 2 The Mars Soil - A Semi-infinite Model

Boundary conditions and initial conditions for the concentration c_i must be specified before equation 15 can be solved. The initial condition is simply $c_i = 0$ at $t = 0$ for $x > 0$ where c_i denotes the exhaust gas concentration within the soil and $t = 0$ is the time at which the exhaust gases initially come into contact with the surface.

Boundary conditions (i.e. surface conditions as a function of time) are a little more difficult to specify since the exact details of the exhaust gas flow field are unknown. However, consideration of the modes of descent of the spacecraft will assist in specifying approximate boundary conditions. According to the work statement of the contract, two descent modes each with two engine cut-off heights are to be considered: (1) a vertical descent case (stationary surface stagnation point) with engine cut-offs at (a) five feet, and (b) twelve feet, (2) a slant descent case such that the surface stagnation point moves at a constant velocity of five feet per second and, again, engine cut-offs at (a) five feet, and (b) twelve feet. During the early phases of the work on this contract, JPL instructed that forty feet* be used as the height of the spacecraft when the exhaust gases first contact the Mars surface, and that a vertical descent velocity of five feet per second be used for both the vertical descent mode and the slant descent mode.

For a vertically descending spacecraft, the exhaust gas concentration at some point on the surface of the far region can be approximated as shown in Figure 3 where $t = 0$ corresponds to the time at which the spacecraft reaches a forty foot height in its descent, and t_1 corresponds to the time at which the engine cut-off height is reached.

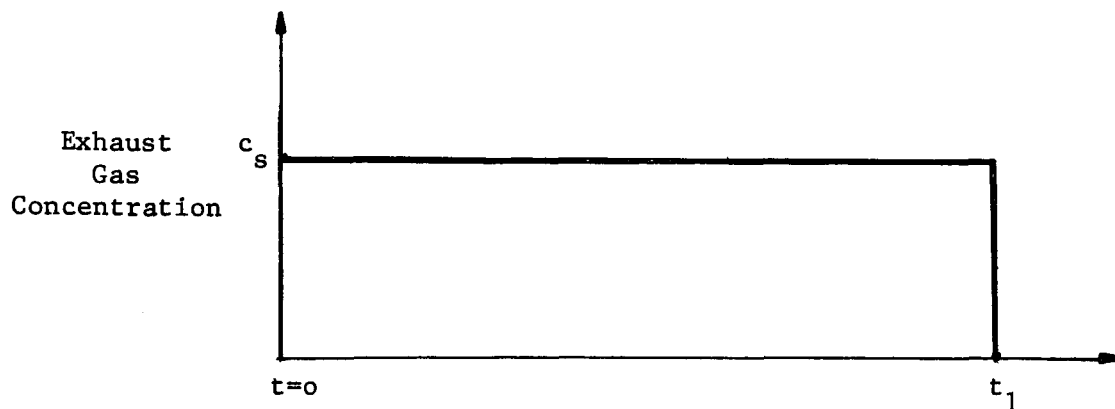


Figure 3 Rectangular Wave Boundary Condition Approximation

*At forty feet, the spacecraft descent trajectory is such that the vehicle should be in a vertical orientation. That is, the engine exhaust will be directed vertically downward from that height down. This is the approximate description for both the vertical descent mode and the slant descent mode.

Other approximate boundary conditions which reflect the more probable gradual changes in the exhaust gas concentration at a general point in the far field are indicated in Figures 4 and 5.

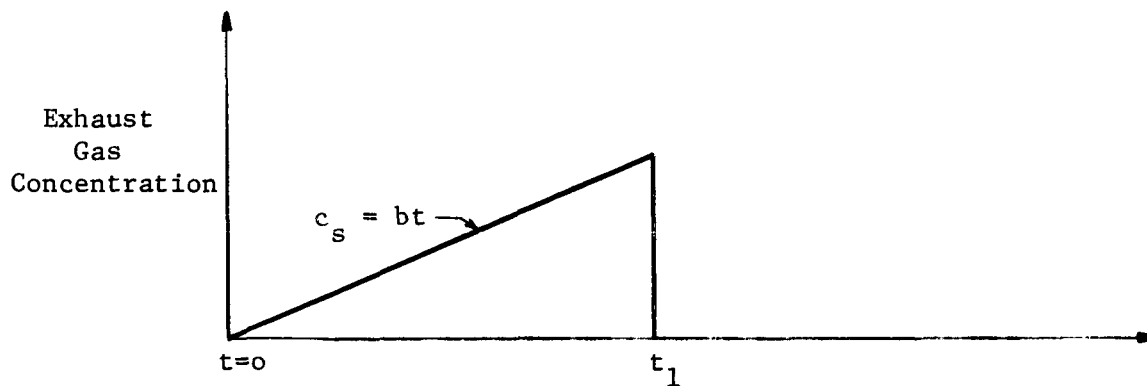


Figure 4 Saw-Tooth Wave Boundary Condition Approximation

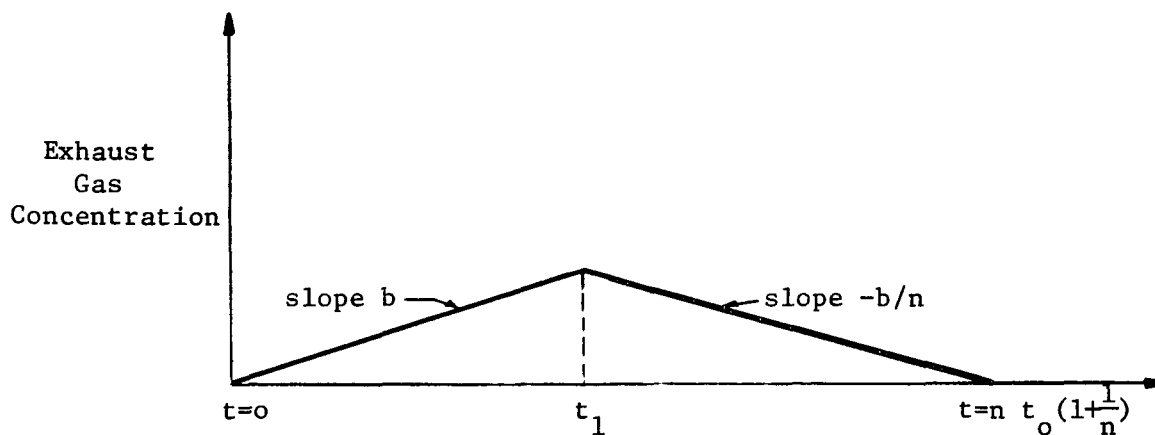


Figure 5 Triangular Wave Boundary Condition Approximation

Times $t = 0$ and $t = t_1$ correspond to the forty foot height time and the engine cut-off time, respectively. Solutions of equation 15 for the boundary conditions above will follow after a discussion on the numerical values of the transport coefficients.

The boundary conditions for the spacecraft slant descent mode differ from those for the vertical descent mode. Since the stagnation point moves along the surface at five feet per second for the duration of the flow, a point initially in the far field region (i.e. at the time the spacecraft is at the forty foot height) may experience the near field condition of total pressure increase before the engine cuts off. Figure 6 indicates the pressure versus time for a point, initially in the far field region, which the spacecraft passes directly over.

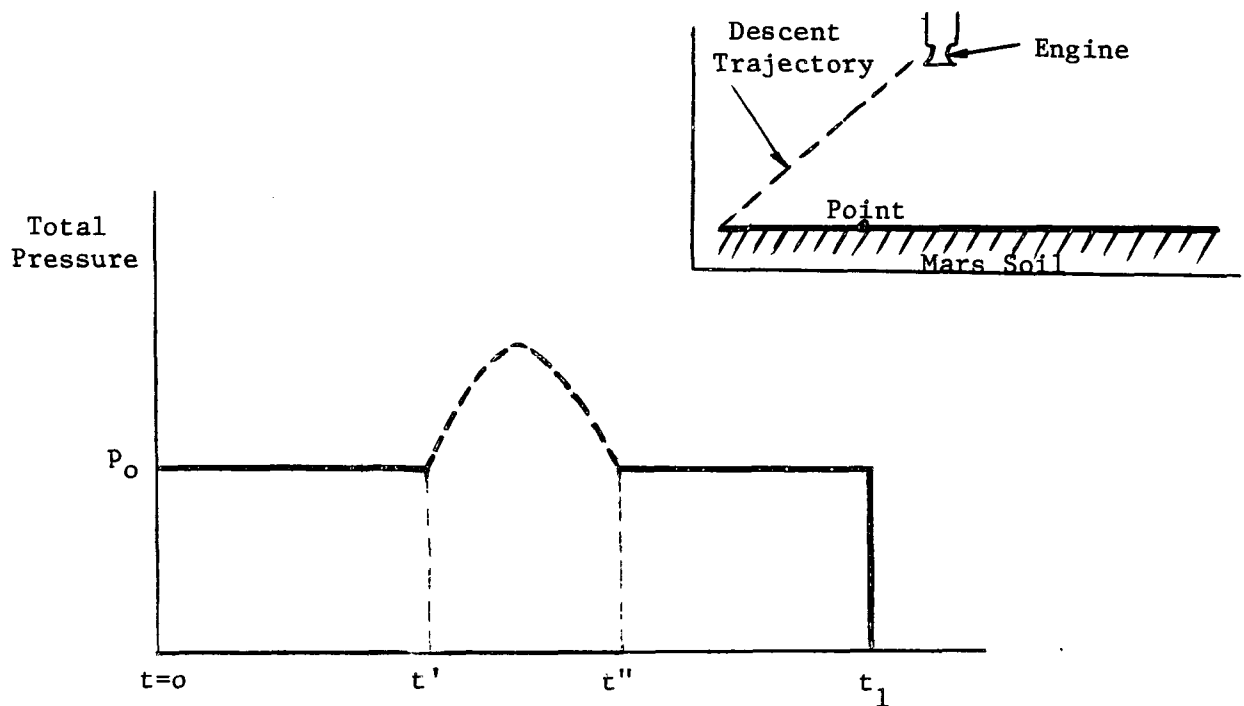


Figure 6 Slant Descent Boundary Condition for a Point Initially in the Far Field

The pressure p_0 denotes the ambient atmospheric pressure, and as explained previously the exhaust gases in the far field have essentially expanded to the pressure p_0 . Therefore, the surface point referred to in Figure 6 is subjected to exhaust gases at pressure p_0 from $t = 0$ to $t = t'$. Then, for the time that it takes the stagnation point to traverse a distance of $20 r_e$ (the approximate near field diameter), the point is subjected to the rapidly changing near field pressures. During the near field period ($t'' - t'$) the gas flow into the soil must be described by equation 11, the nonlinear differential equation requiring a computer solution. The time which the point is exposed to the near field pressure is, however, small compared to the total exposure time t_1 . This near field period ($t'' - t'$) is approximately 1.6 sec ($20 r_e$, where $r_e = 0.389$ ft, divided by 5 ft/sec) whereas the value of t_1 is 5.6 sec for a 12 ft cut-off height, or 7.0 sec for a 5 ft cut-off height. The near field time period of 1.6 sec applies only if the spacecraft passes directly over the point in question. If the descent path (shown in the insert of Figure 6) is away from instead of toward the point, then obviously the point will experience only a shortened far field exposure period.

Since a boundary condition such as Figure 6 results in both diffusion and bulk gas flow into the soil, the flow phenomena is more difficult to analyze than bulk flow (Darcy law flow) alone. Bulk flow is not analyzed in this report, as previously noted, because of the computer requirement and also because of the uncertainties concerning the surface pressure distribution in the near field. Therefore, gas flow into the soil resulting from a boundary condition such as Figure 6 is also not analyzed.

3.3.2 Boundary and Initial Conditions for Heat Flow

The reasoning that led to the simplification of the gas diffusion equation to a one-dimensional form (i.e. a function of only depth into the soil and not radial distance) also applies to the heat transfer equation, equation 7. One therefore obtains

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \quad (16)$$

where $\alpha = k/\rho c_p$. The parameter α is known as the thermal diffusivity and is a property of the material, in this case, the Mars soil.

To obtain a solution to equation 16, one must specify boundary and initial conditions for the temperature. The most reasonable initial condition appears to be $T = T_0$ at $t = 0$ for $x > 0$, where T_0 is assumed a constant independent of depth, $t = 0$ is the time hot rocket gases begin to contact the surface, and $x > 0$ denotes the region beneath the soil surface. Boundary conditions similar to those for the exhaust gas concentration can be applied (Figure 3, 4, 5). However, the magnitudes (i.e. amplitudes of the curves of Figures 3, 4, 5) are not known. If no heat were conducted into the soil (that is, if an adiabatic wall were assumed), one could then calculate the steady state surface temperature by compressible gas flow theory. However, it is inconsistent to first assume an adiabatic surface in order to calculate the surface temperature and then to use this temperature as a boundary condition controlling the flow of heat into the soil. Solutions to equation 16 will be obtained for unspecified magnitudes of surface temperature but with time relationships as given in Figures 3, 4, and 5.

3.3.3 Values of the Transport Parameters

Numerical values of the thermal diffusivity and the diffusion coefficients are reported in this section. First consider the thermal diffusivity α which appears in all solutions of the transient heat conduction equation. An effort

was made, via a search of the literature, to obtain a proper numerical value of α for the Mars soil model*. The search yielded no data for the exact Mars soil constituents, but from a consideration of the range of values of α for Earth soils at low interstitial gas pressure, a prediction of the value of α for the Mars soil model was arrived at.

Values of α are seldom reported in the literature, but values of k , ρ , and c are often given. Therefore, from the definition of α ($\alpha = k/\rho c$), values of α can easily be calculated. Experimentally determined values of k , ρ , and c are of primary interest. Several equations have been proposed to analytically determine the thermal conductivity of a porous medium if the conductivities of the solid phase and the fluid phase (the gas or liquid within the institial pores) are known. However, a difficulty arises in the assignment of the proper value to k_s , the conductivity of the solid component. The conductivities k_f of all the fluid saturants of interest are well known, but there is some doubt as to the conductivity attributable to the solid component. Wechsler and Glaser (6) note that the variation of data for any particular rock type is almost as great as that between different materials. In view of the uncertainty inherent in these emperical expressions, it is best to use direct experimental data.

Of the three parameters, k , ρ , and c , needed to calculate the thermal diffusivity, k varies over the widest range. The soil composition, temperature, and the gas pressure within the pores affect the value of k . Temperature has only a small effect on the value of k . Woodside and Messmer (7) report the values of k for unconsolidated sands as the pore gas pressure is decreased. The thermal conductivity of quartz sand, porosity of 59%, particle size 0.104-0.074 mm, is given at pressures from one atm to 10^{-4} atm. At an air pressure of 10^{-2} atm (approximate Martian Atm. pressure) the value of k is approximately 2×10^{-4} cal/cm sec C. This sand, with the exception of the chemical composition, most closely matches the JPL specified soil model (porosity of 50%, particle size 0.050 mm). Therefore, 2×10^{-4} cal/cm sec C appears to be the proper value of the thermal conductivity to be used in calculating α .

*Based on recent observations of the lunar soil, JPL specified in Technical Direction Memorandum No. 2 that the following minerals be used as the Mars soil model: Quartz - 6.78%, Albite - 22.53%, Anorthite - 25.62%, Diopside - 17.03%, Hyperstene - 20.55%, other - 7.5%, all percentages by weight. Assume a porosity of 50% and an average particle size of 0.050 mm.

The values of ρ and c do not vary considerably from one soil type to another, nor is there a large variation with temperature and pore gas pressure. Values of 1 gm/cm^3 for ρ and 0.2 cal/gm C for c are appropriate for most soil types. Using the values above for k , ρ , and c , the thermal diffusivity is found to be equal to $10^{-3} \text{ cm}^2/\text{sec}$. One should designate this as the expected value for the Mars soil. However, it is possible that α may range from $10^{-4} \text{ cm}^2/\text{sec}$ to $10^{-2} \text{ cm}^2/\text{sec}$ due primarily to the fact that k can vary over two orders of magnitude as the soil composition and gas pressure vary over possible ranges.

Numerical values must now be specified for D_{im} , the diffusion coefficient that appears in equation 15 (the governing expression for the distribution of exhaust gases in the soil). First, consider the values of diffusion coefficients for two component gas mixtures in the absence of a porous medium. Table 1 (compiled from data in references 3 and 8) and the accompanying equation (8) allows one to calculate the diffusion coefficients for the indicated gases at various temperatures and pressures (restricted to the low density regime).

Table 1 Examples of Binary Diffusion Coefficients

for	$D_o \text{ cm}^2/\text{sec}$	m
$\text{H}_2 - \text{N}_2$	0.674	1.75
$\text{O}_2 - \text{N}_2$	0.181	1.75
$\text{H}_2 - \text{Air}$	0.611	1.75
$\text{CO}_2 - \text{O}_2$	0.139	2.00
$\text{H}_2\text{O} - \text{Air}$	0.22	1.75
$\text{CO} - \text{CO}_2$	0.137	-
$\text{CO}_2 - \text{Air}$	0.138	-
$\text{CO}_2 - \text{N}_2$	0.144	-
$\text{Ar} - \text{O}_2$	0.20	-
$D = D_o \left(\frac{T}{T_o} \right)^m \frac{P_o}{P} \quad \text{where } T_o = 273 \text{ K}$ $P_o = 1 \text{ Earth Atm}$		

At a temperature of 273 K and a pressure of 10^{-2} atm (the approximate conditions on the surface of Mars), one obtains diffusion coefficients of one hundred times those values listed in Table 1 as D_0 . Note that with the exception of those gas mixtures one of which is H_2 , the values of the diffusion coefficients vary only over a small range - from 0.14 to 0.22 cm^2/sec , approximately.

The gases which will interdiffuse in the Mars soil are the exhaust gases and the gases comprising the Mars atmosphere. Table 2 lists the gases, and their mole fractions, which comprise the engine exhaust mixture (as given in the contract). The Mars atmosphere is composed primarily of N_2 with a lesser amount of CO_2 - or such is the opinion of most of those dealing with the subject of Mars in the literature (for example, reference 9 and verbal communication with JPL).

Table 2 Exhaust Products

Exhaust Products	Mole Fraction
CO	0.05
CO_2	0.12
H_2	0.26
H_2O	0.26
N_2	0.31

For the exhaust gases paired with one another or with N_2 (with the exception of H_2), the diffusion coefficients should be within the range of values previously extracted from Table 1, namely 0.14 to 0.22 cm^2/sec .

In section 2.3 the multicomponent diffusion process was simplified to a binary diffusion process by the definition of the diffusion coefficient D_{im} . It was noted that if all the diffusion coefficients, D_{ij} , for the various pairs of gases in the multicomponent mixture are equal, then it is correct to set D_{im} equal to D_{ij} . Now, the binary diffusion coefficients of the gases diffusing in the Mars soil are expected to have values in the range 0.14 to 0.22 cm^2/sec ; hence one may assume them equal each with the common value of 0.2 cm^2/sec at one Earth atm or 20.0 cm^2/sec at 10^{-2} Earth atm (the Mars atmospheric pressure is approximately 10^{-2} Earth atm.).

Essentially then, by the above argument, the problem of multicomponent diffusion in the Mars soil has been reduced to the problem of exhaust gas (a single component) diffusing into the soil initially containing atmospheric gases (a single component, N_2) within the pores. This approach should yield reasonable predictions of the exhaust gas concentration as a function of time and depth into the soil. It is likely however that H_2 will diffuse into the soil faster than the bulk of the exhaust gas since the binary diffusion coefficients for gas pairs, one of which is H_2 , is several times larger than the diffusion coefficients for the gases involved in this study. It does not follow that H_2 will diffuse into the soil at a rate proportional to the diffusion coefficient of H_2 into N_2 . This is due to the presence of the other gases and to the assumption regarding the equality of diffusion coefficients (which allowed the D_{im} approach).

The "average" diffusion coefficient value of $20 \text{ cm}^2/\text{sec}$ referred to previously must first be modified to account for the presence of the soil before using it in the diffusion equation, equation 15. With a porous medium present, the normal diffusion coefficient should be multiplied by the factor ϵ/τ where ϵ is the porosity and τ is the tortuosity factor* of the soil (10). However, the left hand side of equation 15 should be multiplied by the porosity ϵ to account for the fraction of open volume. Since ϵ now occurs on both sides of the equation, one simply obtains

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} \quad (17)$$

where $D = D_m/\tau$. The subscripts on c and D have been deleted; c now denotes the concentration of the exhaust gas considered as one component, and D_m denotes the effective binary diffusion coefficient, with the value $20 \text{ cm}^2/\text{sec}$, for the exhaust gas diffusing into the low pressure Mars atmospheric gas (considered as a single component). Division of D_m by the tortuosity factor accounts for the soil's presence. The tortuosity factor is approximately 1.5 for nearly all random-packed porous materials (11). Therefore, for diffusion in the Mars soil, D equals $(20/1.5) \text{ cm}^2/\text{sec}$, or $13.5 \text{ cm}^2/\text{sec}$.

*The soil porosity ϵ is defined as the ratio of pore volume to total volume. The tortuosity factor is defined as the ratio of the actual distance the gas traverses in diffusing from one point to another to the straight line distance between the two points in the porous medium.

A discussion of the value of the diffusion coefficient will not be complete until rarefied gas diffusion is considered. Basically, three diffusion regimes may be defined: (1) the continuum regime, (2) a transition regime, and (3) the rarefied (Knudsen flow) regime. According to Scott and Dullien (10) continuum flow occurs for $r/\lambda > 10$, where r is the "average" pore radius and λ is the mean free path length of the gas molecules, the transition regime is encountered for $0.1 < (r/\lambda) < 10$, and Knudsen flow occurs for $r/\lambda < 0.1$. These r/λ ranges have not been thoroughly verified, and some disagreement exists in the literature.

The relations expressing the diffusion coefficient as a function of temperature, pressure, molecular weight, etc., differ for each of the three regions. For example, the equation contained in Table 1 is valid only for the low density continuum regime (perfect gas regime). The diffusion coefficient for Knudsen flow is approximately $(2/3) r \bar{v}$ for porous materials where \bar{v} is the average molecular velocity (12). Several empirical relations exist for the transition regime coefficient. For example, Rothfeld (13) obtained the expression

$$\frac{1}{D_T} = \frac{1}{D_K} + \frac{1}{D_B} \quad (18)$$

where D_T , D_K , and D_B refer to the transition, Knudsen, and continuum diffusion coefficients, respectively.

With regards to exhaust gas diffusion in the Mars soil, it appears that the diffusion mechanism may be in the upper transition regime. At a 10 millibar pressure, the typical exhaust gas molecule has a mean free path length of approximately 10 microns. The pore size within a medium composed of 50 micron diameter particles (JPL Technical Direction Memorandum No. 2 specified a uniform 50 micron particle size for the soil model) can not be uniquely specified, yet the pore size is obviously less than the particle diameter. Assuming a pore size of 10 microns, and using proper values of the other parameters, equation 18 yields a transition diffusion coefficient of approximately $10 \text{ cm}^2/\text{sec}$ (instead of $13.5 \text{ cm}^2/\text{sec}$ for the continuum regime). In conclusion, the continuum regime coefficient will be retained for application since compared to the transition coefficient it is a "worst case," and since effective pore size is not known.

3.3.4 Specific Solutions to the Heat Transfer and Diffusion Equations

The equations finally arrived at for the prediction of heat transfer and gas diffusion into the Mars soil, repeated below, are:

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \quad (16)$$

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} \quad (17)$$

Best estimates of the thermal diffusivity α and the effective binary diffusion coefficient D were determined to be $10^{-3} \text{ cm}^2/\text{sec}$ and $13.5 \text{ cm}^2/\text{sec}$, respectively. The boundary conditions most likely to be experienced for the vertical descent mode are suggested in Figures 3, 4, and 5. For the slant descent mode a boundary condition arises, Figure 6, which can not be imposed upon equation 17 (this equation describes flow due to concentration gradients only and not total pressure gradients).

Note that equations 16 and 17 have the same form but different dependent variables and transport coefficients. One may therefore expect the general solutions of the two equations to be similar. By the methods of Laplace transforms, the general solution to equation 17 for the semi-infinite soil model and for an arbitrary time varying boundary condition is easily obtained as

$$c(x,t) = \int_0^t c_s(\tau) \frac{x}{\sqrt{4\pi D}} \frac{\exp[-x^2/4D(t-\tau)]}{(t-\tau)^{3/2}} d\tau \quad (19)$$

where $c_s(t)$ is the time varying boundary condition. The solution to equation 16 differs only by the term accounting for the initial temperature T_0 (the initial conditions for the two equations were previously specified as a zero concentration of exhaust gas in the soil and a uniform temperature T_0 in the soil). Therefore, for the solution to equation 16 one obtains.

$$T(x,t) - T_0 = \int_0^t T_s(\tau) \frac{x}{\sqrt{4\pi \alpha}} \frac{\exp[-x^2/4\alpha(t-\tau)]}{(t-\tau)^{3/2}} d\tau \quad (20)$$

where $T_s(t)$ is the time varying temperature boundary condition.

The integral term of equation 19 and 20 may be analytically evaluated for certain functional forms of $c_s(t)$ and $T_s(t)$.

For boundary conditions sketched in Figures 3, 4, and 5, the results are .

a)

$$\frac{c}{c_s} = \operatorname{erfc} \frac{x}{2\sqrt{Dt}} - \operatorname{erfc} \frac{x}{2\sqrt{D(t-t_1)}} \quad (21)$$

for the boundary condition (corresponding to Figure 3)

$$c_s = \begin{cases} c_s, & 0 < t \leq t_1 \\ 0, & t > t_1 \end{cases}$$

b)

$$\begin{aligned} \frac{c}{c_{s \max}} = & \left(\frac{t}{t_1} + \frac{x^2}{2Dt_1} \right) \left(\operatorname{erf} \frac{x}{\sqrt{4D(t-t_1)}} - \operatorname{erf} \frac{x}{\sqrt{4Dt}} \right) \\ & + \frac{x}{t_1\sqrt{\pi D}} \left[\sqrt{t-t_1} \exp -x^2/4D(t-t_1) - \sqrt{t} \exp -x^2/4Dt \right] \end{aligned} \quad (22)$$

where $c_{s \max} = bt_1$, and for the boundary condition (corresponding to Figure 4)

$$c_s = \begin{cases} bt, & 0 < t \leq t_1 \\ 0, & t > t_1 \end{cases}$$

c)

$$\begin{aligned}
\frac{c}{c_{s \max}} = & \frac{1}{t_1} \left(1 + \frac{1}{n} \right) \left[\left(t + \frac{x^2}{2D} \right) - t_1 \right] \left[\operatorname{erf} \frac{x}{\sqrt{4D(t - t_1)}} \right] \\
& - \left(\frac{t}{t_1} + \frac{x^2}{2Dt_1} \right) \left(\operatorname{erf} \frac{x}{\sqrt{4Dt}} \right) \\
& + \frac{1}{t_1} \left[\left(1 + \frac{1}{n} \right) t_1 - \frac{1}{n} \left(t + \frac{x^2}{2D} \right) \right] \left[\operatorname{erf} \frac{x}{\sqrt{4D[t - (n+1)t_1]}} \right] \\
& - \frac{x}{t_1} \sqrt{\frac{t}{\pi D}} \left(\exp - x^2/4Dt \right) \\
& + \frac{1}{t_1} \left(1 - \frac{1}{n} \right) \left(x \sqrt{\frac{t - t_1}{\pi D}} \right) \left[\exp - x^2/4D(t - t_1) \right] \\
& - \left(\frac{x}{t_1} \sqrt{\frac{t - (n+1)t_1}{\pi D}} \right) \left(\exp - x^2/4D[t - (n+1)t_1] \right) \quad (23)
\end{aligned}$$

where $C_{s \max} = bt_1$, and the boundary conditions (corresponding to Figure 5)

$$c_s = \begin{cases} bt & , \quad 0 < t < t_1 \\ -(b/n)t + (1 + \frac{1}{n}) bt_1 & , \quad t_1 < t < t_1(n+1) \\ 0 & , \quad t > t_1(n+1) \end{cases}$$

An approximate solution of equation 19 may be obtained for values of time large compared to the time at which the surface concentration goes to zero. Denote the time at which the surface concentration goes to zero as t_f (t_f corresponds to t_1 in Figure 4 and 5, and $nt_0(1 + \frac{1}{n})$ in Figure 5). Then, for $t \gg t_f$, equation 19 reduces to

$$c(x,t) = \frac{x}{\sqrt{4\pi D}} \frac{t_f}{t^{3/2}} \exp(-x^2/4Dt) \frac{\int_0^{t_f} c_s(\tau) d\tau}{\int_0^{t_f} d\tau},$$

$$c(x,t) = \frac{x}{\sqrt{4\pi D}} \frac{t_f}{t^{3/2}} \exp(-x^2/4Dt) (c_s)_{\text{avg}},$$

or

$$\frac{c(x,t)}{(c_s)_{\text{avg}}} = \frac{x}{\sqrt{4\pi D}} \frac{t_f}{t^{3/2}} \exp(-x^2/4Dt) \quad (24)$$

where $(c_s)_{\text{avg}}$ is simply the time averaged surface concentration.

As explained in Section 3.3.2, the temperature boundary conditions should be approximately the same as the exhaust gas concentration boundary conditions. Therefore the same functional relations (equations 21, 22, 23, and 24) also are valid expressions for $(T - T_o)/T_s$ once α is substituted for D .

Selected curves representing the exhaust gas concentration profiles are shown in Figures 7, 8, and 9. In each figure, the curve intersecting the ordinate at 1.0 represents the concentration profile at engine cut off time. Curves could be plotted for times less than the engine cut off time. Such curves would still intersect the ordinate at 1.0, but the concentration would decrease more quickly with depth. After engine cut off, the surface concentration of exhaust gas returns to zero, and therefore for times greater than the engine cut off time, the curves intersect the ordinate at 0. Exhaust gas begins to diffuse out of the soil as soon as the engine cuts off, and the exhaust gas concentration at all depths therefore decreases with time. Note that the diffusion out of the soil is also quite rapid. After approximately one minute the concentration c/c_s at any depth is generally less than 0.05.

Temperature profiles were not plotted because the value of $[T(x,t) - T_o]$ approaches zero very quickly with increasing depth x . For example, for the rectangular wave boundary condition of Figure 3 using $t_1 = 7$ sec, the value of $(T - T_o)/T_s$ at $x = 1$ cm is less than 0.01 for any time t . Thus, as a result of the small value of the thermal diffusivity and the short time which the surface is heated by the exhaust gases, only the soil within one centimeter of the surface is appreciably heated. That is, near the surface ($x < 1$ cm), $(T - T_o)/T_s$ varies rapidly from 1.0 to less than 0.01, and for $x > 1$ cm, $(T - T_o)/T_s$ remains less than 0.01 for all time t .

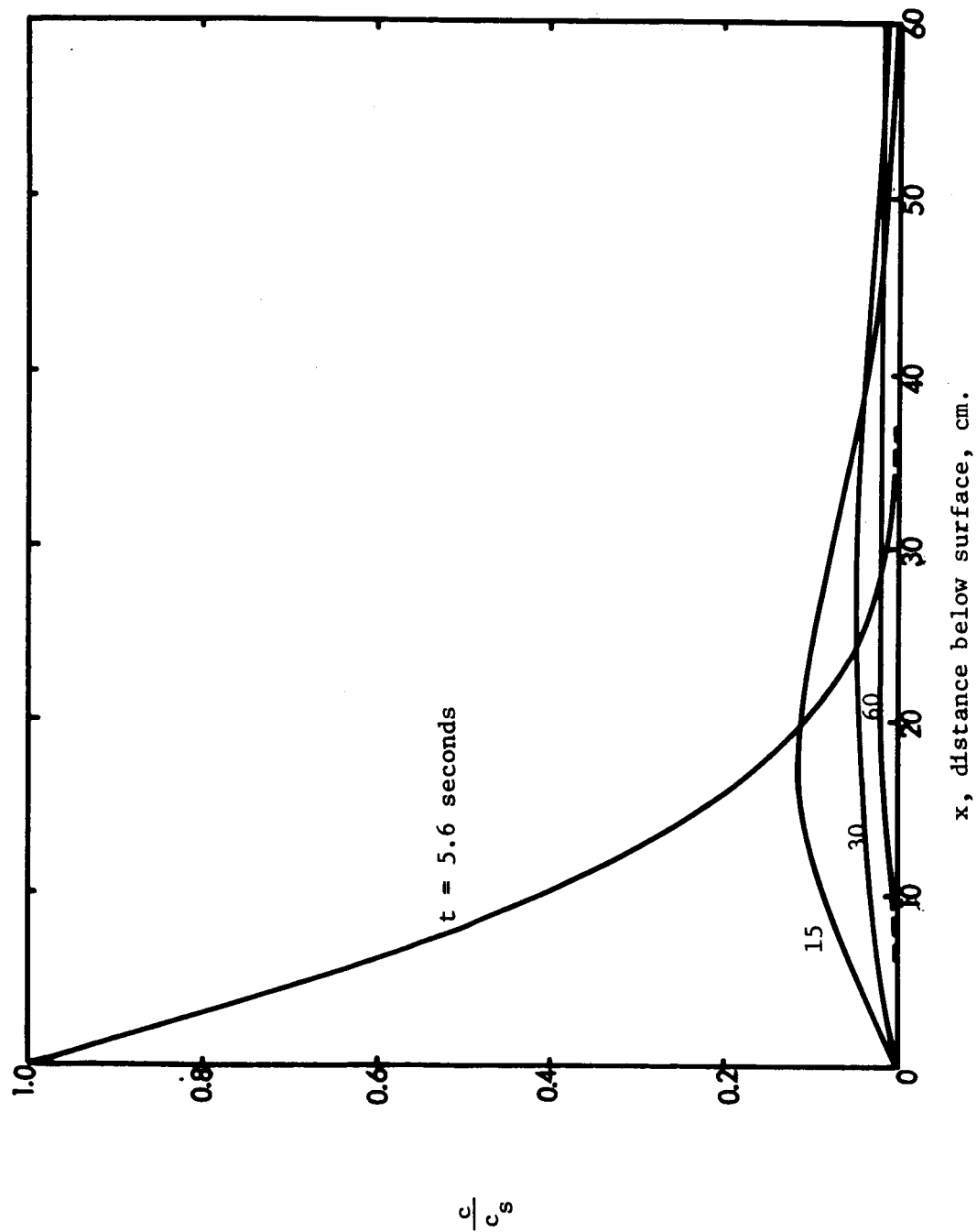


Figure 7 Concentration Profiles Resulting from a Rectangular Wave Form Boundary Condition with Engine Cutoff at 5.6 seconds.

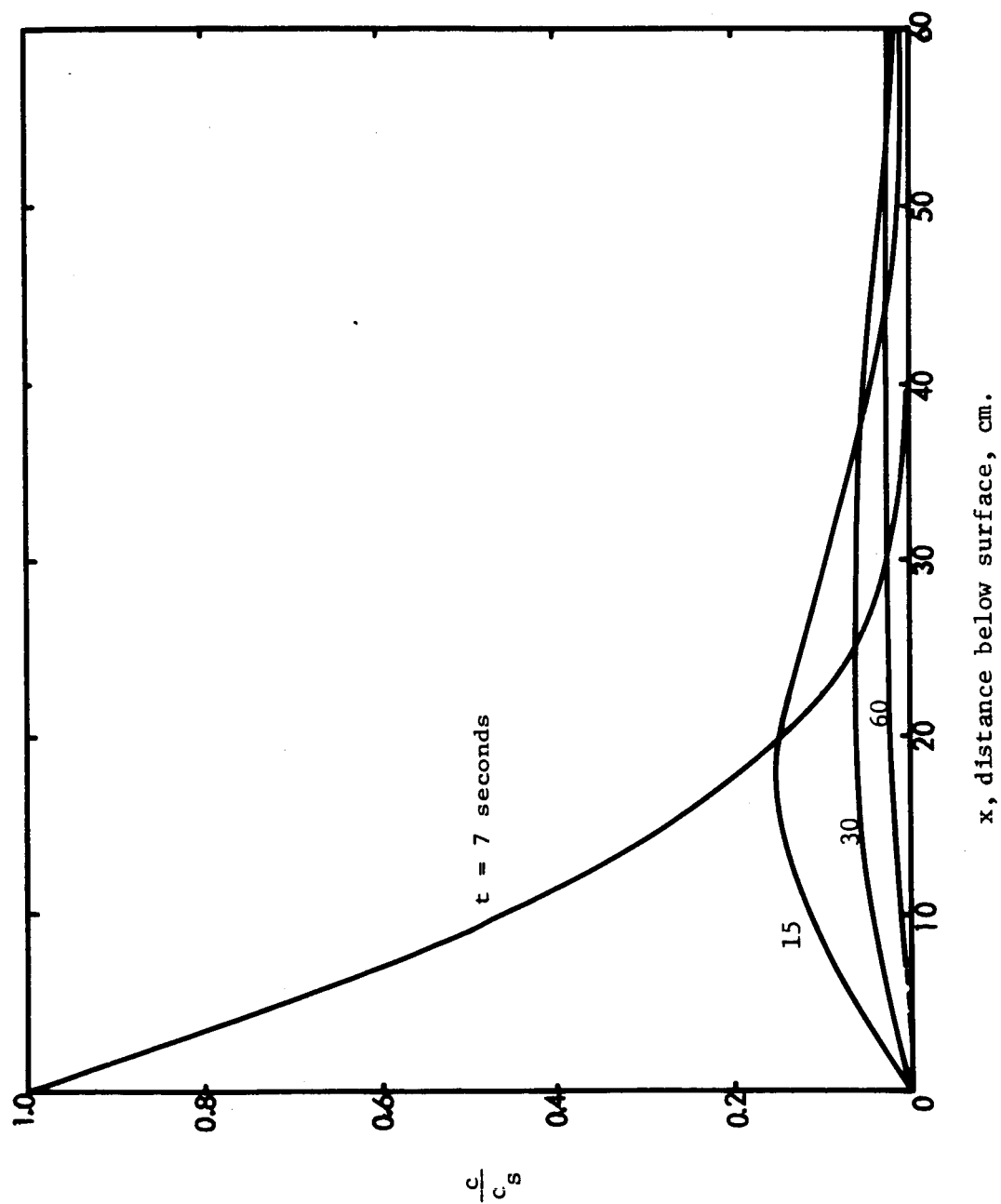
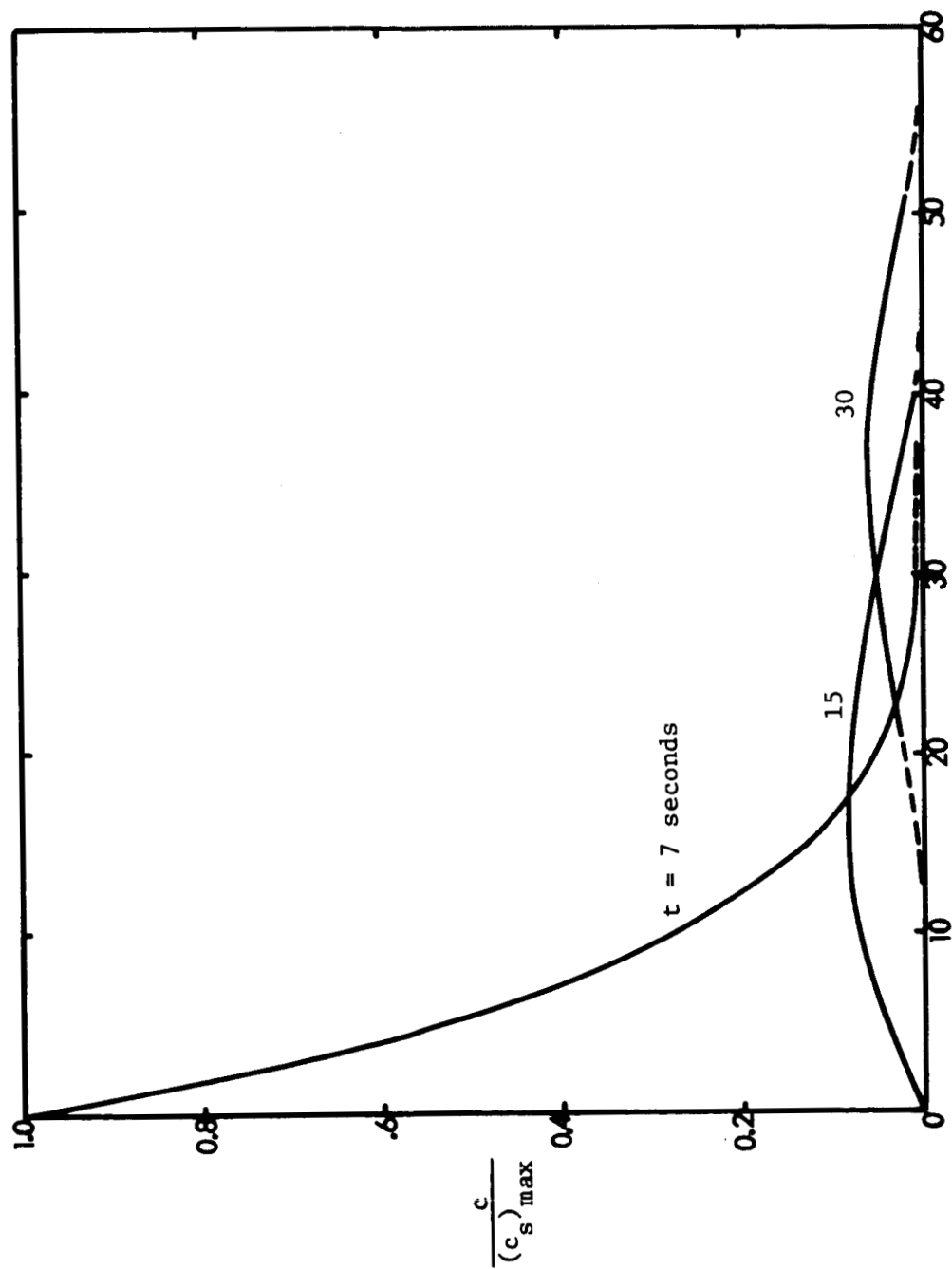


Figure 8 Concentration Profiles Resulting from a Rectangular Wave Form Boundary Condition with Engine Cutoff at 7.0 seconds.



x , distance below surface, cm.

Figure 9 Concentration Profiles Resulting from a Triangular Wave Form Boundary Condition with Engine Cutoff at 7.0 seconds.

One may now justify the assumption made earlier that the temperature gradients should affect the gas flow only to a small degree. That is, the gas diffuses into the soil at a much higher rate than the heat is conducted into the soil. Thus, except very near the surface, the gas diffuses through soil at a temperature T_0 , the initial temperature. To show that this is true, note that the solutions of equations 19 and 20 contain x , and D or α always as x^2/D or x^2/α . Thus, for a specific time t , c/c_s and $\Delta T/T_s$ have the same numerical values at different depths x_c and x_T , respectively, where the x_c and x_T are related as

$$\frac{x_c^2}{D} = \frac{x_T^2}{\alpha},$$

or

$$\frac{x_c}{x_T} = \sqrt{\frac{D}{\alpha}}$$

From values of D and α previously obtained ($D = 13.5 \text{ cm}^2/\text{sec}$, $\alpha = 10^{-3} \text{ cm}^2/\text{sec}$) one obtains $x_c/x_T \approx 100$, or $x_c \approx 100 x_T$. In other words, the "wave front" representing gaseous diffusion has proceeded, at any time t , to a depth about 100 times the depth of the temperature "wave front."

3.3.5 Simultaneous Diffusion and Adsorption

As exhaust gas diffuses into the Mars soil, selective adsorption of the exhaust gas constituents by the soil particles may occur. Now, two types of adsorption are possible. Physical adsorption of a particular specie by a surface tends to take place simply through forces of physical attraction similar to those causing the deviations of real gases from ideal laws, the liquefaction of gases, etc. On the other hand, chemical adsorption resulting from the formation of strong chemical bonds between the adsorbent and the adsorbate may occur. Generally speaking, the adsorbed component has a finite average "lifetime" with the result that a desorption process also occurs. A steady state condition is reached whenever the desorption rate equals the adsorption rate.

There is no sharp demarcation between physical adsorption and chemical adsorption, yet general distinctions have become obvious (14). The heat of adsorption for chemical bonds is normally an order of magnitude greater than for physical bonds. Physical adsorption generally takes place at much lower temperatures than chemisorption. Chemisorption, being a chemical reaction, may require an appreciable activation energy whereas physical adsorption requires no activation energy. Chemisorption depends upon the adsorbent surface being clean, and even then not all clean surfaces are active in chemisorption. Physical adsorption takes place on all surfaces under the correct conditions of temperature and pressure. Chemisorption ceases when the adsorbate can no longer make direct contact with the surface and is therefore a single molecular layer process. With physical adsorption no such limitation applies, and under suitable conditions of temperature and pressure, physically adsorbed layers many molecules thick can be obtained.

After studying the factors controlling adsorption processes, it appears that few conclusions can be reached regarding the probability of physical and/or chemical adsorption of constituents of the exhaust gas mixture by the Mars soil model assumed. Too many unknowns exist. The initial soil temperature and the extent of surface heating by the exhaust gas must be known precisely. The prior amount of adsorption of Mars atmospheric gases by the soil is important since it relates to the "cleanliness" of the soil (as noted above, chemical adsorption is very much dependent upon the soil particle surface conditions). Even if all temperatures, pressures, and surface conditions were determined, a mathematical analysis of the transient adsorption-desorption processes would not be possible simply because very little experimental data is available concerning the rates at which adsorption and desorption of gases by solids takes place. Some adsorption data exist for the equilibrium state of gases in contact with solids. Such data are usually presented as adsorption isotherms; that is, curves of mass adsorbed versus gas pressure. Rate coefficients can not be deduced from equilibrium data, unfortunately, and since the exhaust gas-soil interaction is a relatively fast transient process, equilibrium adsorption data are of no use.

Aronowitz, et al. (1) in their investigation of lunar surface contamination were also handicapped by lack of relevant data on adsorption and desorption. After considerable discussion and presentation of a simple theory to calculate

the average lifetime of various chemisorbed gases on silicate rock, it was concluded that the theory allowed at best only rough order of magnitude estimates of the lifetimes. Calculations were also presented on the "sticking coefficient" (actually the adsorption probability) of gases impinging on the lunar surface. However, the final conclusion of the report was that to determine the distribution of adsorbed exhaust gas on the lunar surface it is necessary to know the rates of adsorption and desorption; experimental data are needed since almost no reliable data are otherwise available.

Even though the necessary adsorption and desorption rates for exhaust gases in the Mars soil are not presently available, solutions of equations 13 and 14 have been obtained (for a special case). If adsorption and desorption rates become available in the future, these solutions will prove useful. First, consider the derivation of equation 13 and 14. Adsorption and desorption may be accounted for by including appropriate "source" and "sink" terms in the diffusion equation (equation 12) for each component of the gaseous mixture. Thus,

$$\frac{\partial c_i}{\partial t} = D_m \frac{\partial^2 c_i}{\partial x^2} + \lambda_d c_{di} - \lambda_c \left(1 - \frac{c_{di}}{C_{di}}\right) p$$

where c_i is the concentration of the i^{th} gas. The product $\lambda_d c_{di}$ is the source term and accounts for the desorption process; c_{di} is the concentration of adsorbed gas and λ_d is the reciprocal lifetime for desorption with the product $\lambda_d c_{di}$ having dimensions of particles (or mass) per unit time per unit volume of soil. This source term $\lambda_d c_{di}$ reflects the assumption that desorption is proportional to the number of particles previously adsorbed. The product $\lambda_c [1 - (c_{di}/C_{di})] p$ is the sink term and accounts for the adsorption process. The absorption rate is proportional to the rate at which molecules strike the surface of the soil particles, and this is proportional to the pressure -- hence the factor p in the product above. Also, the adsorption rate is proportional to the degree of previous adsorption. To reflect the previous adsorption, let c_{di} be the adsorbed concentration at any time and C_{di} be the saturation value of c_{di} . Thus $[1 - (c_{di}/C_{di})]$ represents the surface area fraction not yet covered. The factor λ_c is a proportionality constant with dimensions of particles (or mass) per unit time per unit volume per unit pressure. This model of surface adsorption is patterned after the well-known Langmuir model.

A second equation is required - a conservation equation for the adsorbed gas, c_{di} , namely,

$$\frac{\partial c_{di}}{\partial t} = \lambda_c \left(1 - \frac{c_{di}}{C_{di}}\right) p - \lambda_d c_{di}$$

In both equations, p may be replaced by $c_i kT$ since $p = c_i kT$ for a perfect gas where k is Boltzman's constant. Both equations above are nonlinear, but if $c_{di}/C_{di} \ll 1$ (adsorption not near the saturation value) then the expressions may be linearized. Redefining λ_c as $\lambda_c = kT\lambda_c$ and neglecting c_{di}/C_{di} , one obtains equations 13 and 14 given previously,

$$\frac{\partial c_i}{\partial t} = D_m \frac{\partial^2 c_i}{\partial x^2} + \lambda_d c_{di} - \lambda_c c_i \quad (13)$$

$$\frac{\partial c_{di}}{\partial t} = \lambda_c c_i - \lambda_d c_{di} \quad (14)$$

A general solution to these equations can be found by the method of Laplace transforms, however, the resulting integrals are complex and difficult to work with. A more practical approach is to note that the physically interesting case is when the adsorption rate is quite rapid and the desorption rate is slow. One may then neglect the term $\lambda_d c_{di}$ in equation 13. The term is retained in equation 14 in order to assure the correct asymptotic behavior of c_{di} for large times.

With the term $\lambda_d c_{di}$ in equation 13 neglected, the solutions of equations 13 and 14 are found to be

$$c_i(x,t) = \frac{x}{\sqrt{4\pi D_m}} \int_0^t c_{si}(\tau) \frac{\exp[-\lambda_c(t-\tau) - x^2/4D_m(t-\tau)]}{(t-\tau)^{3/2}} d\tau \quad (25)$$

and

$$c_{di} = \int_0^t c_i(x,\tau) \exp[-\lambda_d(t-\tau)] d\tau \quad (26)$$

4. SUMMARY AND RECOMMENDATIONS

The findings of this analytical study on the transport of heat and rocket engine exhaust gas into the Mars soil are reviewed in this section.

Since the heat and gas transport predictions are very dependent on the differential equations chosen to model the transport processes, it was necessary to give considerable attention to the proper formulation of the governing equations. The Mars surface region exposed to exhaust gases was separated into a near field region and a far field region based on the total pressure distribution. Heat and mass transport equations were developed for each region, but simplifying assumptions were necessary to obtain equations amenable to solution. Heat transfer into the soil of both regions is primarily by conduction and not by convection; hence convection is neglected. Mass transport is assumed to be independent of temperature gradients in the soil.

Gas flow into the soil of the near field region (that surface area within a distance of ten nozzle exit radii from the flow field stagnation point) is governed by a nonlinear differential equation which requires a numerical solution. A solution to this equation was not obtained for several reasons:

(a) the total pressure varies rapidly with time and position in the near field area -- such a boundary condition complicates any solution, (b) the near field area is actually quite small (approximately a four foot radius disk about the stagnation point) and is thus not extremely important, and (c) obtaining any numerical solutions to the nonlinear equation would have likely required significant computer time and expense.

Gas flow into the soil of the far field region (that surface area beyond a distance of ten nozzle exit radii from the flow field stagnation point) was analyzed in detail. Concentration gradients are the primary driving force for diffusion into the soil of the far field region since the total pressure remains at the ambient. The set of diffusion equations, one for each gas diffusing in the multicomponent mixture, can not be solved because the numerous diffusion coefficients are unknown. Analytical methods simply can not be employed for transient, multicomponent diffusion problems where the number of gases in the mixture exceeds three. Therefore, the problem of exhaust gas diffusing into the soil initially containing Mars atmospheric gases in the pores was simplified

to a binary diffusion problem. The exhaust gas, considered as one component of a binary mixture, was assumed to diffuse into the soil initially containing Mars atmospheric gas, the second component.

Solutions to the diffusion equation were obtained utilizing proper values of the effective diffusion coefficient and reasonable boundary conditions. The boundary conditions were chosen with consideration to the rate of descent of the spacecraft. The results indicate that diffusion of gas into the soil is significant only to a depth of approximately 30 centimeters below the surface. Below 30 centimeters, the maximum concentration of exhaust gases is approximately 0.1 that at the surface. Generally speaking, diffusion into the soil surface is subjected to exhaust gas flow for only a short period of time (less than 10 sec). Thus, a significant quantity of exhaust gas does not have time to diffuse into the soil before the engine shuts down. The exhaust gas that does diffuse into the soil also rapidly diffuses out of the soil once the engine cuts off. Calculations show that after as short a time as 60 seconds, the amount of exhaust gas remaining in the soil is negligible.

The extent of adsorption of exhaust gases by the Mars soil remains unknown. Absence of experimental data on adsorption and desorption rates precludes a quantitative analysis to determine the amounts of exhaust gases, if any, that are adsorbed in the soil. Since information on the adsorption-desorption phenomena is necessary for a thorough knowledge of the contamination effects of exhaust gas on the Mars soil, it is recommended that an experimental effort be considered to determine adsorption and desorption rate coefficients in various soil models. Since primary interest presently lies in the question of exhaust gas water vapor adsorption (or condensation, which is simply a physical adsorption process) by the soil, experimental emphasis should be placed on the water vapor adsorption-desorption process. A soil model can be placed in a container which is then evacuated to the approximate atmospheric pressure on Mars. The soil temperature also should be controlled by heating or cooling coils. Then, adsorption and desorption processes may be initiated by injecting water vapor in controlled amounts into the container. The recorded pressure versus time data may be correlated with simple adsorption-desorption mathematical models in order to determine adsorption and desorption rate coefficients. These coefficients may then be utilized in the differential equation governing gas diffusion with simultaneous adsorption and desorption in the Mars soil.

If interests in the near field soil contamination problem increases, then it is also suggested that an experimental program be undertaken to measure exhaust gas pressure at the soil surface as a function of time and distance from the stagnation point. The gas flow into the soil in the near field area is caused by the changes in total pressure at the surface and is described by a nonlinear differential equation. Precise knowledge of the rapidly varying pressure conditions at the surface will allow a computer solution of the governing equation.

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